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Small Angle X-ray Scattering on Diamond

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Abstract

Building of the new UK Diamond synchrotron at the Rutherford Laboratory is now well advanced and beamlines are being assembled. Here progress on the non-crystalline diffraction facilities I22 (being implemented) and HATSAX (possible) is outlined, together with plans for on-line data analysis.

Update on Beamline I22

[1] Optics Design

Design work for the optics hutch is nearing completion with only some diagnostic components still outstanding. Initial beam diagnostics will be performed by a pair of FMB designed X-ray photon beam position monitors (Figure 1). These will be installed into I22's front end and will give the beamline an accurate indication of incident beam position and stability.

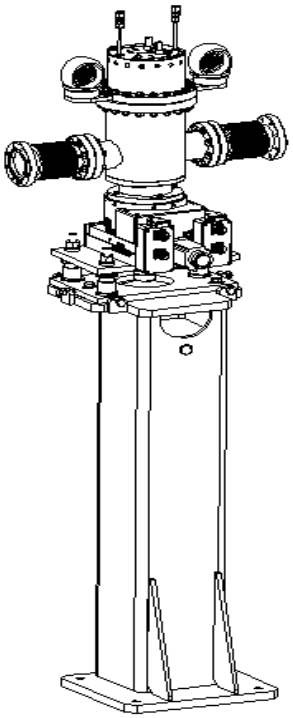

Figure 1 *- FMB XBPM, two will be installed into I22's front end giving information on beam position and angle.*

In the optics and experimental hutches the diagnostics will comprise both beam observation and measurement through in-house designed diagnostic systems (Figure 2). In time these will be incorporated into the feedback systems for I22 to ensure that the user community get optimum performance from the beamline.

Figure 2 *- Monochromatic beam Diagnostic assembly. This will give information about position, intensity and shape of the beam incident through the optics on I22.*

[2] End Station

The end station design is progressing well with contracts let for the Sample platform (IDT - Figure 3a) and detectors (HOTSAXS, HOTWAXS and RAPID with CCLRC). The Small Angle X-ray Scattering Detector mounting platform will allow both detectors to be available to the user community during a scheduled experiment with minimal changeover time (Figure 3b). The HOTWAXS detector will be mounted on an A-frame above orbit plan, the nosecone for the detector has been designed such that alternative front pieces can be mounted to minimise air gaps for different sample environments.

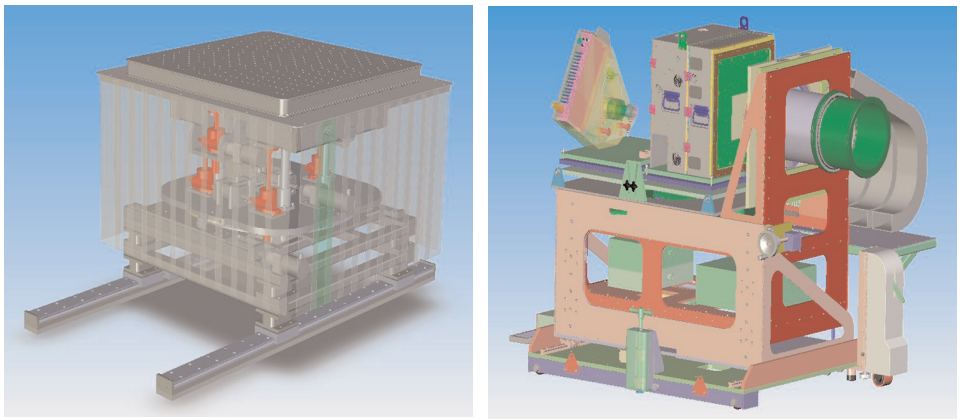

Figure 3 *- Left) Sample platform with breadboard for easy mounting of sample environments. This assembly is also adaptable to include spacers to vary the height of the platform grossly. Right) Small Angle X-ray Scattering Detector platform. Also included on this assembly is the beamstop. Independent movement of detector and beamstop is possible.*

The beamline compliment of sample environments will be discussed over the coming months but is likely to include DSC, capillary heater, stop flow cells and liquid cells. Sample changers can be accommodated on the standard sample platform and users are encouraged to contact the beamline team to discuss their requirements at the earliest possible convenience. The sample platform has x-y translation (±100mm) and limited pitch (±5°) and yaw (±10°) for sample alignment purposes.

[3] Building I22

IDT designed the primary silts for I22 (Figure 4). These are at Diamond Light Source and are ready to be installed once the cabins and services contract is complete.

The monochromator from Oxford Danfysik is due for delivery in April. The characteristics of the fixed exit monochromator will allow I22 to deliver anomalous scattering experiments in the range 4-20keV without the need for translation of the sample stage.

The K-B mirror system from Accel has been delivered and will be installed in the optics hutch towards the middle of May this year. The properties of the vertical focusing mirror (VFM) have been tested at Elettra (Figure 5) and indicate that I22 will have excellent performance from its focusing system (slope error <1.3?m without bimorph correction).

The monochromatic slits have also been delivered to Diamond Light Source (Figure 6). We have worked with ADC to produce a design that should, not only act as an excellent slit system (blade roughness <1?m), but also provide feedback. The blades have been electrically isolated and therefore it should be possible to measure beam position via a drain current measurement. This information can again be fed back to the optics system to ensure stable sampling.

[4] Installation of I22

Anyone who has been to Diamond over the last 12 months will have seen that tremendous progress has been made on all fronts. I recommend that anyone interested takes a look at http://www.diamond.ac.uk/default.htm regularly. I22 is also taking shape. On the experimental floor the x-ray hutches have been installed and we are nearing the completion of the cabins and services installation (Figure 7).

Figure 4 *- Left) Primary Slits Assembly. Right) one of the water cooled blades prior to assembly.*

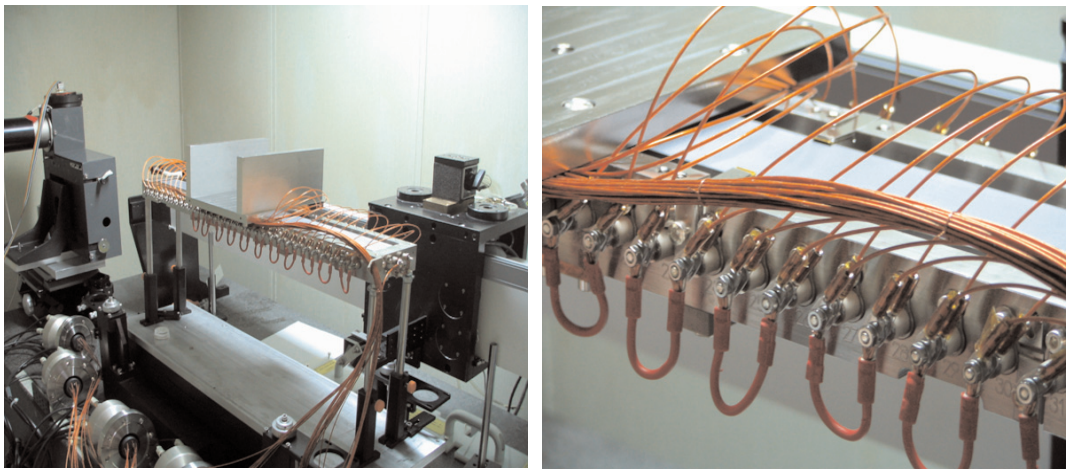

Figure 5 *- Two views of the VFM for I22 during testing at Elettra. The pictures give a view of the 32 electrode connections. For these tests they were shorted together.*

Figure 6 *- Monochromatic slits 2, you can see the electrical feed through's alternately spaced with the motor mechanism around the flange into which the slits are mounted..*

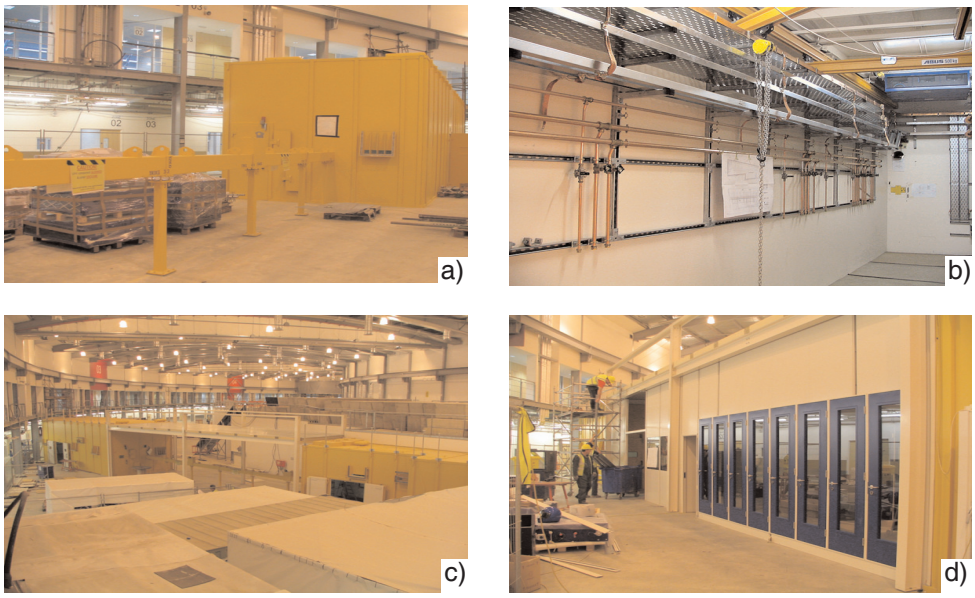

Figure 7 *- Views of I22 during installation a)Transfer line showing Experimental hutch, b) internal detail of Optics hutch showing tray work and services supply pipes, c) Overview of I22 area, optics hutch to right and experimental hutch to left. Installation of the steel-work to support the user and control cabins is underway in the middle d) View showing the Controls and Instrumentation Area (CIA) areas and in back-ground the User cabin..*

The CIA will house the control racks for motors, vacuum and data handling. Regular photographic updates of construction progress can be found at: http://www.diamond.ac.uk/Beamlines/Beamlineplan/I22/Progress.htm.

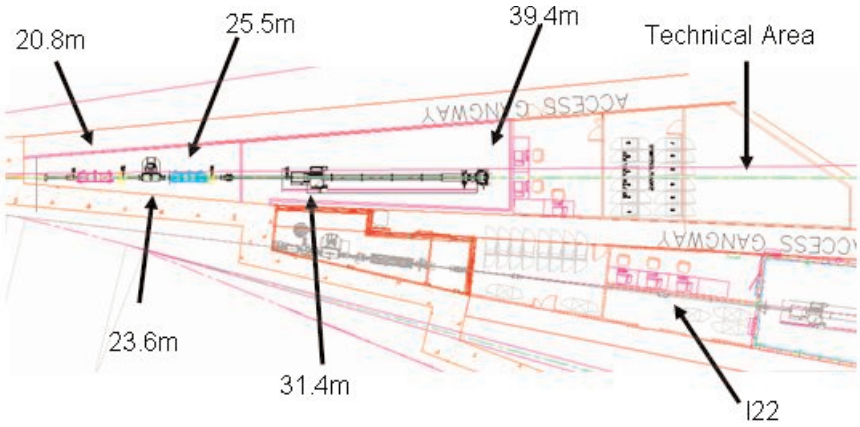

Figure 9 *Possible layout for HATSAXS alongside I22.*

[5] Commissioning of I22

Commissioning with X-rays will commence later this year after the installation of our U25 in-vacuum undulator in August. Commissioning without beam is expected to be an ongoing process as soon as the first equipment is installed in June 2006.

[6] Data reduction - Data Analysis

It will be possible to carry out data reduction on line for both 1D and 2D data on I22. Building on the GDA software that is being rolled out across all Diamond beamlines we have developed simple data reduction screens that will take the users through the basic steps, data normalisation, detector response correction and experimental background subtraction. Working with live data from the current experiment and using only a few parameters that can be adjusted it will give a very quick view of the data so that decisions can be made during beamtime rather than offline later. These simple mode screens are complimented by a scripting engine that will permit more complicated operations to be performed. Figure 8 shows two screenshots for the package. Figure 8a illustrates how simple mode for 1D data will look. The illustration has 100 curves of simulated scattering intensity from spheres of different diameters. Figure 8b illustrates how the 2D display will look. The illustration here displays the same 1D data as in Figure 8a displayed as a 2D plot but could be of any 2D data set. It is planned to "pipe" the data from these programs into any user community data analysis packages including all of those from CCP13.

Progress on developing a HATSAXS on Diamond

There is a proposal to build a second beamline for Small Angle X-ray Scattering (HATSAXS) on Diamond using a bending magnet source. If all goes well the beamline will be operational by 2011. The layout in Figure 9 shows how a possible HATSAXS solution may look on the Diamond experimental floor. It will be located alongside I22 to allow the two beamlines to share resources.

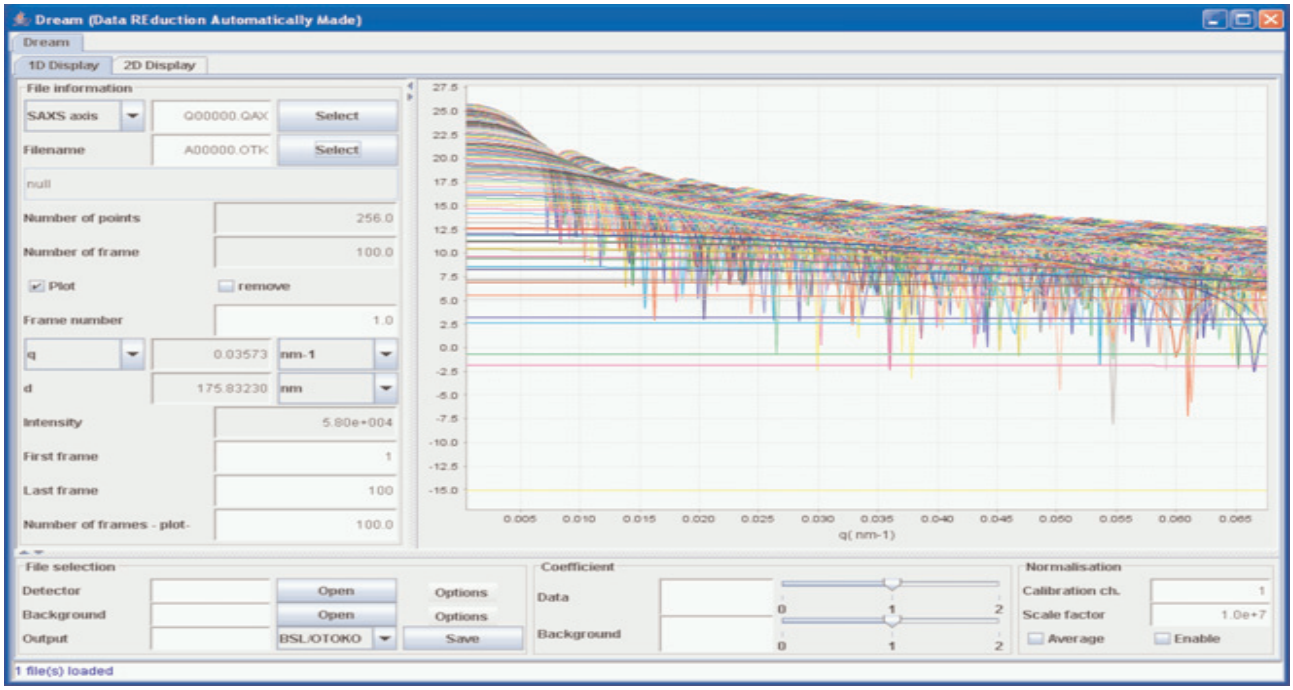

Figure 8a*: shows the envisaged 1D panel.*

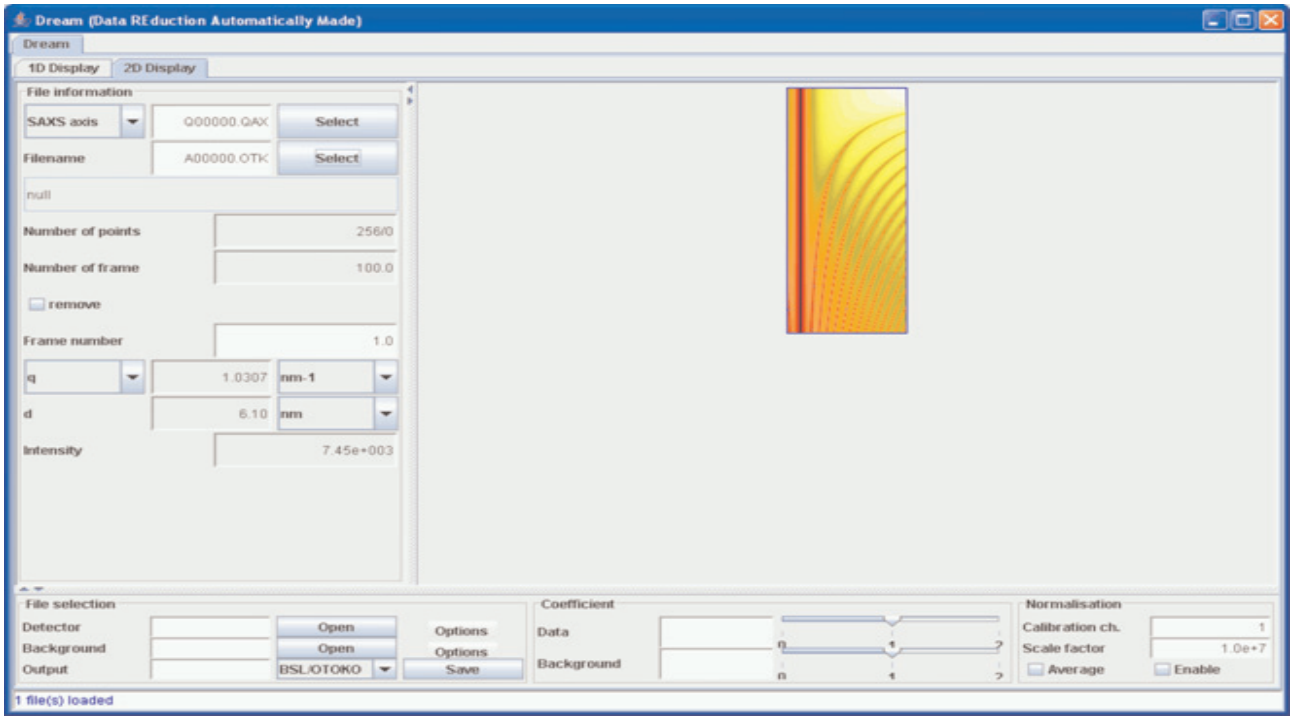

***Figure 8b**: shows the envisaged 2D panel*

	SRS line6	**Diamond dipole 2:1**	**Diamond dipole 3:1**
Source	10 pole MPW 2.0T	Dipole 1.4T	Dipole 1.4T
Mirror length	1.2m	1.2m	1.2m
Mirror width	0.14m	0.14m	0.14m
Horizontal fan	1mrads	0.6mrads	0.6mrads
Vertical fan	0.35mrads	0.35mrads	0.35mrads
X-ray energy	10keV	10keV	10keV
Beam current	200mA	300mA	300mA
Mirror slope error	0.5 arc-sec FWHM	0.5 arc-sec FWHM	0.5 arc-sec FWHM
Sagittal crystal thickness variation	15% over 60mm	15% over 60mm	15% over 60mm
Focal spot size sigma (HxV) at 10keV	0.42mm x 0.09mm	0.07mm x 0.06mm	0.05mm x 0.07mm
Focal spot divergence sigma (HxV) at 10keV	0.60mrad x 0.23mrad	0.39mrad x 0.16mrad	0.59mrad x 0.27mrad
Flux in focus	3.6 x 10^{12} photons/sec	2.1 x 10^{12} photons/sec.	2.1 x 10^{12} photons/sec

***Table 1** - Performance Comparison for SRS line 6 with Diamond Dipole at 2:1 and 3:1 demagnification*

Table 1 shows the possible performance of a beamline built this way. The flux is down on the comparable beamline, 6.2, at the SRS, but beamsize and divergence are also smaller.